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Comparisons of Line Emission from ICF Capsules in 2- and 3-Dimensionsal Simulations

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**Abstract**--Hydrodynamic instabilities reduce the yield in inertial confinement fusion (ICF) implosions. Line emission from dopants placed in the capsule can be used to diagnose the extent of the instabilities. This paper presents the results of a large number of 2D simulations and a few 3D simulations of line emission from argon in the DH fuel and titanium placed in the inner layers of the plastic shell of a NOVA ICF capsule. The simulations have been compared to NOVA experimental data on the ratio of argon Ly-$\beta$ to titanium He-$\alpha$, the relative strength of titanium He-$\alpha$ and its satellites, and the strength of the continuum near titanium He-$\alpha$. The simulations are in reasonable agreement with the data, but the amount of data is small enough that it is hard to make precise comparisons. Two different atomic databases have been used in a first attempt to determine the set of configurations required to properly model the titanium emission.

*Keywords*: Radiative Transfer; Inertial Confinement Fusion; Atomic Line Emission

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## 1. INTRODUCTION

Mix due to hydrodynamic instabilities is important in inertial confinement fusion (ICF) implosions because it reduces the thermonuclear yield. One technique for studying these instabilities is to measure the line emission of dopants placed in the fusion capsule. In the simulations discussed here, titanium was placed in the inner layers of the plastic shell and argon was placed in the DH fuel. Titanium emission is weak if the implosion is symmetric (all the plastic remains cool). If the interface between the fuel and the plastic shell becomes highly distorted, titanium emission increases as parts of the shell push inward into the hottest parts of the fuel. Line emission from titanium is thus a signature of a distorted shell. The temperature of argon drops and its line emission decreases when the interface becomes highly distorted.

In earlier papers [1,2,3,4,5], we presented the first models of line emission from ICF capsules based on 2D and 3D simulations that included radiative transfer of atomic lines. Those papers may be consulted for more details about the modeling process. This paper extends our earlier results by considering the coupled effects of capsule surface roughness and x-ray drive asymmetry in two dimensions. The

2D simulations cover the range of initial capsule surface roughness and x-ray drive asymmetry present during the HEP-4 series of NOVA experiments (ref??). A few three dimensional simulations have been run to assess whether the response to surface roughness depends on dimensionality. Future simulations will address the coupled effects of surface roughness and x-ray drive asymmetry in three dimensions.

## 2. THE MODELING PROCEDURE

The 2D results presented in this paper come from a simulation of an ICF capsule that has both angular variations in the x-ray drive radiation and perturbations on the initial capsule surface. The capsule is shown in Fig. (1). The capsule is driven by x-rays generated in a hohlraum like those used in Nova experiments (see Lindl [6] for a discussion of the Nova laser facility). The capsule has germanium in the outer portion of the plastic shell to absorb hard x-rays and prevent preheat of the plastic. Titanium is placed in the innermost part of the plastic shell and argon is placed in the DH fuel. The titanium and argon concentrations are low enough that they do not change the implosion hydrodynamics.

Angular variations in the x-rays and bumps on the plastic shell are a source for hydrodynamic instabilities. These perturbations grow on the outer surface due to the Rayleigh-Taylor instability [7] [8] during the inward acceleration of the capsule and feed through to perturb the inner surface. Perturbations at the inner surface grow due to the Rayleigh-Taylor instability when the shell decelerates at the time of peak compression. Richtmeyer-Meshkov instabilities [9] [10] occur as shocks pass through the capsule and serve as a seed for Rayleigh-Taylor instabilities.

The hohlraum is driven by a 2.0 ns laser pulse with 32 kJ of 0.35 μm light. There is an intensity contrast of 5 between the low intensity foot of the pulse and the main drive x-rays. The radiation drive asymmetry is based on experimentally measured beam-to-beam power imbalances and pointing errors as well as the intrinsic time-dependent P2 and P4 drive asymmetries in the hohlraum [11]. To provide the asymmetric x-ray drive for a particular simulation, a set of random numbers is used to choose specific beam pointing errors from the experimental distribution. This is combined with time-dependent P2 and P4 asymmetries from a 2D Lasnex [12] simulation to generate an angle- and time-dependent x-ray source. The 2D simulations performed for this paper used several different drive asymmetries for each initial surface roughness. The 3D simulations include initial surface roughness but use a symmetric drive.

Line emission is modeled by first running a radiation-hydrodynamics code to compute time-dependent temperatures and densities. Lasnex was used for 2D simulations and HYDRA [13] was used for 3D simulations. Cretin [14] used the temperatures and densities from the rad-hydro code (2D and 3D) to solve the kinetics equations for the populations of the atomic configurations simultaneously with the radiation transport equations for the Helium- and Lyman-$\alpha$ lines. All other lines were assumed to be optically thin.

The Lasnex 2D simulations were run on two processor Pentium 4 Linux computers. Seven different initial surface roughnesses ranging from 0.013 μm to 0.7 μm were used. For each surface roughness, five different drive asymmetries were used (the same 5 were used for all surface roughnesses). The Lasnex grid covered a hemi-sphere and had 150 azimuthal points and 140 radial points. The Lasnex models used four carefully chosen frequencies with mean opacities that were calculated from a 1D implosion run with many frequency groups [15]. Lasnex has a Langrangean hydrodynamics package, but the simulation was rezoned to an orthogonal grid whenever grid distortions became large.

The HYDRA 3D models were run on ASCI white, a large IBM SP-2 system at LLNL. The HYDRA simulation used 166 radial zones, 64 azimuthal zones, 32 zones in polar angle, and covered two octants. The HYDRA models used three carefully chosen frequencies with mean opacities that were calculated from a 1D implosion run with many frequency groups [15]. The HYDRA simulation used an orthogonal grid whose radial zoning follows the motion of the shell. HYDRA has an interface tracker to avoid numerical diffusion of material at the boundary between the fuel and the shell.

Cretin simulations were run for all 2D simulations. The 2D Cretin simulations were run on a single alpha Linux processor. Cretin simulations have only been completed for a subset of the HYDRA runs. The 3D Cretin simulations require 17 GB of memory when run on 2 processors and were run on HP/Compaq alpha systems.

For the 3D simulations, Cretin used an atomic database from the Ration code [16]. This database has a total of 70 configurations, with most of the configurations devoted to hydrogen-like, helium-like and doubly excited lithium-like ions. There are also hydrogenic ground-state configurations for less ionized stages.

The high density and relatively low temperature in the region of titanium emission leads to strong satellites to the titanium He-$\alpha$ line. To begin an assessment of the impact of the atomic database on satellite line emission, the 2D simulations used both the Ration database and a database created by Sam Dalhed. Dalhed's database has 395 configurations with many multiply excited helium, lithium, beryllium, and boron-like configurations. Dalhed's database does not currently include LS splitting. In the future we plan to add LS splitting and keep only the important multiply excited configurations. Our goal is to find a database that does a good job of modeling the satellite lines but is still small enough to use in 3D simulations.

The compressed fuel and plastic shell reach electron densities of order $10^{25}$ $cm^{-3}$, so both Stark broadening and continuum lowering are important [17]. Stark broadening is handled by including an appropriate width in the calculation of the Voigt profile for each line. The width is obtained from fits to detailed line shape calculations [18] where applicable, and from theoretical formulas [19] for the remaining lines. Continuum lowering is handled in a Stewart-Pyatt approximation [17] that has been modified so configurations disappear smoothly as the density is varied. These models have 700 or more frequencies in the output spectrum so that the individual lines can be resolved if they do not overlap due to broadening.

The argon Ly- and He-$\alpha$ lines and the titanium He-$\alpha$ lines are optically thick in these capsules. The effects of line trapping are self-consistently included in the line transfer calculation for these lines. All other lines are optically thin and are not transferred. We have not included the continuum opacity of the plastic in these simulations.

## 3. COMPUTATIONAL ISSUES

Cretin has been able to model the transport of line and continuum radiation in two dimensions for several years. The 2D transfer package tracks radiation in three dimensions through a two dimensional grid. We now regard these simulations as routine and at one point were running 90 of them simultaneously.

It was reasonably straightforward to modify Cretin to handle transport through a 3D grid. The greatest difficulty in moving to three dimensions is the large increase in memory and computing time needed to run a simulation. The 3D Cretin simulations presented in this paper had half a million grid cells. At each grid point, the radiation field is computed in 48 angular directions for 60 line energy bins and 70 continuum radiation bins. There are also populations for 74 configurations at each point. The spectrum is computed at 500 frequencies after the populations are determined. There are over 1.5 billion unknowns to be updated at every time step. By sharing work arrays and otherwise carefully conserving memory, we are able to run the problem on two processors in 17 GB of memory. One time step took 12 hours on a 1 GHz Compaq alpha es45 (this computer has 32 GB of memory and is the only place we could run these simulation at LLNL).

The memory per processor can be decreased by decomposing the grid into several domains. Although the aggregate memory requirement increases when this decomposition is made, the simulation will then fit on a number of parallel computers at LLNL. Cretin supports this type of parallelism, but the current scheme is inefficient. For that reason, these simulations were run using shared memory parallelism on the computer with the largest memory available to us.

## 4. RESULTS

The goal of these simulations is to develop a predictive capability for argon and titanium line strengths that will allow us to infer the level of distortion of the interface between the fuel and the plastic shell from measured line emission. The titanium comes from a very thin layer of material on the inside of the shell where the plastic is warm enough for titanium K-shell lines to be emitted. This requires good spatial resolution in the radial direction. The hydrogenic lines of argon come from throughout the DH fuel while the helium-like lines are emitted in the portions of the fuel that are near the shell.

The distortion in the interface between the fuel and the shell ranges from modest for capsules with smooth initial surfaces to very large for the capsules with the largest initial surface roughnesses. A slice through a 3D capsule with a 0.013 $\mu$m RMS outer surface roughness is shown in Fig. (2) 30 ps after peak compression (most of the lines have been emitted by this time). The distortion in the interface is modest. A slice through the 3D capsule with a 0.1 $\mu$m RMS outer surface roughness is shown in Fig. (3) at the time of peak compression. The capsule already has large distortions at this time.

Figures (4) and (5) compare the 2D and 3D fusion yields to the experimental data. The simulations predict roughly twice as many neutrons as are seen in the experiments, but the dependence on surface roughness is similar. The scatter in the yield is smaller in the 2D simulations for smooth capsules than in the experiments. The yield drops in the simulations when cold material pushes into the fuel and conducts heat out of the fuel. In the 2D simulations an azimuthally symmetric ridge of cold material pushes into the fuel while in 3D simulations a "finger" of cold material is responsible for the drop in yield. Marinak [illegible]believes that the coupling between surface perturbations and drive asymmetries is different in 2D and 3D. He suggests that it is easier for the two processes to couple and drive a single "finger" of plastic into the fuel than it is to drive a "ridge" of shell material into the fuel in 2D. Our 3D simulations cannot yet address this point because we have not included 3D drive asymmetry.

A simulation that matched the experimental yield would have a different distribution of temperatures and densities than the current simulations. In particular, the temperature in the fuel should on average be lower. A simulation that matched the experimental yield would also give different values for the line strengths. We will compare our current simulations to the experimental line emission with the understanding that the results will change by some unknown amount if/when we have simulations that match the yield.

The line emission rates for Ar Ly-β and Ti He-α are shown as a function of time in Fig. (6). The argon Ly-β emission peaks earlier in time (2.01 to 2.03 ns) than the titanium emission (2.05 ns). This difference might be detectable with a streaked spectrometer with a time resolution of roughly 20 ps.

Fig. (7) compares titanium He-α emission obtained with the Ration and Dalhed databases to experimental data for a capsule with 0.013 μm roughness. The simulations using the Dalhed database do not include any continuum radiation to show which spectral regions are dominated by continuum. The Ration simulations significantly over-estimate the continuum. The Ration simulation does a somewhat better job of matching the ratio of He-α to its satellites than the simulation using Dalhed's database. The simulation using the Ration database has satellite lines covering too broad of an energy range. The Dalhed database did not include LS splitting (??), so its energies were adjusted to make the Ti He-α line be at the same energy as it is in Ration and the experiments.

Fig. (8) shows the spectra for a capsule with 0.57 μm roughness and a simulation with 0.7 μm roughness. In this case the Ration spectrum agrees well with the experimental continuum above the line but it overestimates the continuum below the line. Once again, the Ration simulation does a somewhat better job of matching the ratio of He-α to its satellites than the simulation using Dalhed's database. Additional experiments with lower noise levels would help select between the two databases.

Figures (9) and (10) show the time integrated spectrum for capsules with initial surface roughnesses of 0.013 and 0.7 μm, respectively. The strength of the Ar Ly-β line decreases more than the strength of the Ti He-α line as the surface becomes rougher and the continuum emission at the energy of the titanium line drops by over a factor of two.

The ratio of Ar Ly-β to Ti He-α is shown in Fig. (11). The simulations used the Ration database. The simulated ratio decreases rapidly as the surface roughness increases up to 0.5 μm and then appears to flatten after that point. Simulations with a 1.0 μm RMS are planned to confirm the flattening. The simulations are in reasonable agreement with the experimental data. There are only a few experiments and there is a lot of scatter in the ratio for smooth capsules, so it is hard to quantify the level of agreement. The scatter may be due to variations in the experimental conditions (e.g. the total laser energy, the capsule thickness, the capsule radius) that are not accounted for in the simulations.

## 5. CONCLUSIONS

The 2D simulations of the argon Ly-β to titanium He-α ratio are in reasonable agreement with the experimental data. The simulations are also in reasonable agreement on the ratio of TI He-α to its satellite lines. Agreement on the strength of the continuum is not as good, especially to the red side of Ti He-α. Reducing the scatter and noise in the experimental data would permit more sensitive comparisons and in particular might help settle on the importance of the atomic database in predicting spectra. The simulations consistently over-predict the number of fusion neutrons. The 3D simulations did not account for the drive asymmetry. We hope to examine this effect in the future. The 2D simulations include both surface roughness and drive asymmetry. There may be other experimental variations not accounted for in the 2D simulations or the mechanism reducing the yield may have an intrinsically 3D aspect.

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Figure Captions

Fig. (1). The capsule consists of a plastic shell filled with DT gas. The plastic includes germanium to prevent hard x-rays from heating the inner portions of the shell. The inner layer of the plastic has a small amount of titanium and the fuel has a small amount of argon to serve as spectroscopic tracers.

Fig. (2). The density in the xy-plane is shown 30 ps after peak compression. This HYDRA simulation had an initial surface roughness of 0.018 μm RMS. Contour lines show the boundaries of the region that contains titanium. The perturbations are modest at all times with significant line emission for this simulation.

Fig. (3). The density in the xy-plane is shown at the time of peak compression. This HYDRA simulation had an initial surface roughness of 0.1 μm RMS. Contour lines show the boundaries of the region that contains titanium. The perturbations are already large at this time.

Fig. (4). The fusion yield is plotted as a function of initial surface roughness. Some experiments used bromine rather than germanium, but the hydrodynamic performance of the two kinds of capsule should be the same. The simulated yield is roughly a factor of 2 greater than the experiments. The discrepancy may be due to the inability of 2D simulations to correctly model the coupling of perturbations from surface roughness and drive asymmetry.

Fig. (5). The fusion yield is plotted as a function of initial surface roughness. The 3D simulations are shown as a black line and the experimental data is shown by symbols. The simulations are higher than the experiments, but the effects of drive asymmetry have not been modeled.

Fig. (6). Argon Ly-$\beta$ (green) and titanium He-$\alpha$ (black) strengths are shown as functions of time for 7 initial surface roughnesses ranging from 0.013 to 0.7 μm. Both line strengths drop as the surface becomes rougher, but argon drops faster. The ratio of these two lines can thus be used as an indicator of the distortion of the fuel-shell interface. The argon emission peaks roughly 20 ps earlier than titanium for smooth capsules and nearly 40 ps earlier for the roughest surfaces.

Fig. (7). This figure compares time-resolved 2d simulated titanium spectra using the Ration (thick black) and Dalhed (thick dashed) databases to experimental spectra at the time of peak emission for a capsule with initial surface roughness of 0.013 μm. The detector is not absolutely calibrated, so all three curves have been normalized to the same maximum. The Ration simulation agrees with the experimental ratio of the He-$\alpha$ line to its satellites but overestimates the continuum. The satellite lines cover too wide a range of energies. The Dalhed simulations do not include continuum radiation. They agree better with the energy range of the satellites but overestimate the strength of the satellite lines.

Fig. (8). This figure compares time-resolved 2d simulated titanium spectra using the Ration (thick black) and Dalhed (thick dashed) databases to experimental spectra at the time of peak emission for a capsule with initial surface roughness of 0.6-0.7 μm. The detector is not absolutely calibrated, so all three curves have been normalized to the same maximum. The Ration simulation agrees with the experimental ratio of the He-α line to its satellites and with the continuum above the line energy, but it overestimates the continuum below the line. The satellite lines cover too wide a range of energies. The Dalhed simulations do not include continuum radiation. They agree better with the energy range of the satellites but overestimate the strength of the satellite lines.

Fig. (9). The time integrated spectrum for a capsule with an initial surface roughness of 0.013 μm has a titanium line that sits on top of a strong continuum.

Fig. (10). The time integrated spectrum for a capsule with an initial surface roughness of 0.7 μm has a weak continuum at the energy of the titanium line.

Fig. (11). The ratio of Argon Ly-β to titanium He-α is plotted as a function of initial surface roughness. The 2D simulations are shown in blue and the experimental data with error bars is shown in black. The simulated ratio may be slightly higher than the experiments, but there is significant scatter in the experiments. Background subtraction is not handled the same for the simulations and the experiments. Correcting this could shift the ratio significantly.

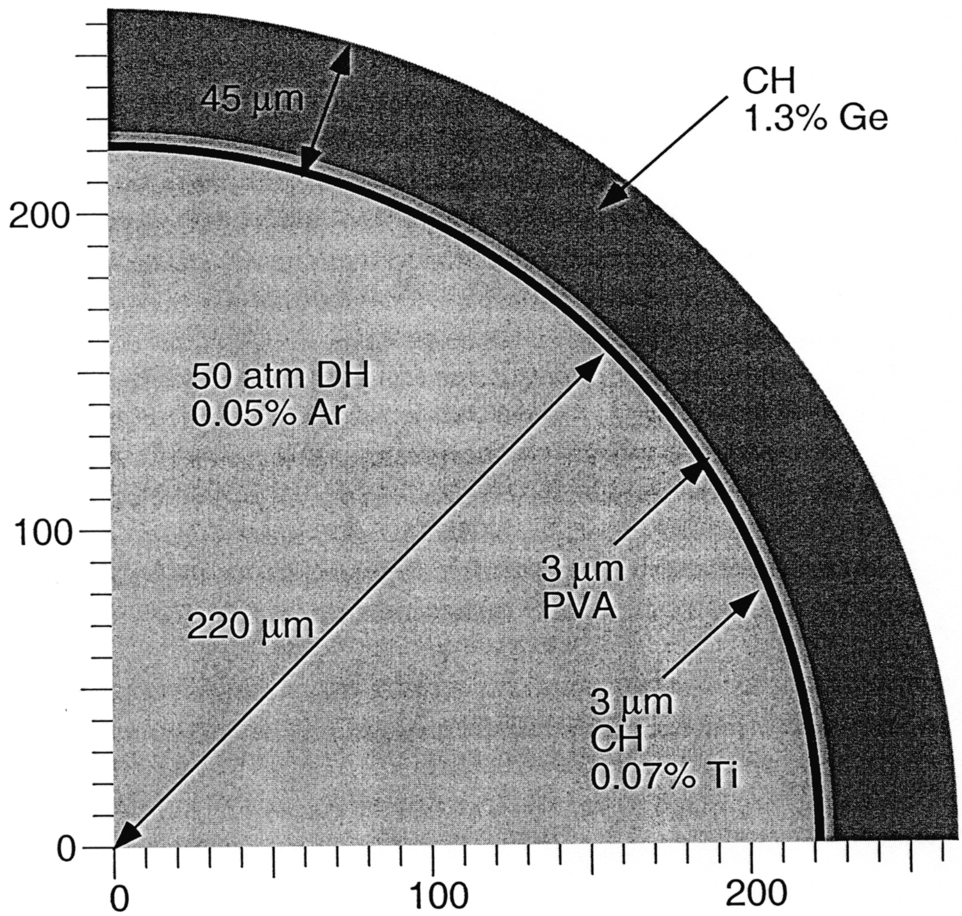
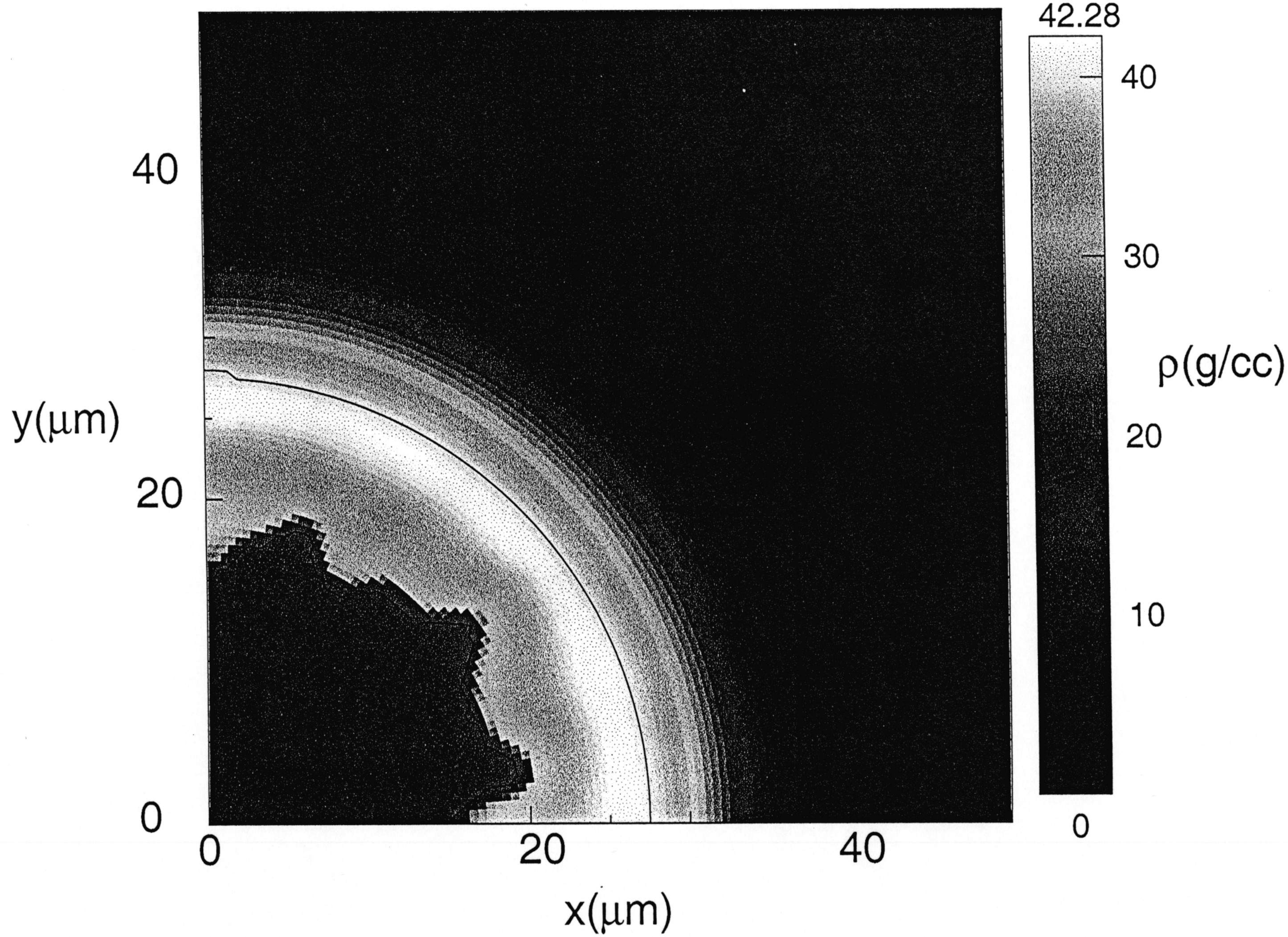
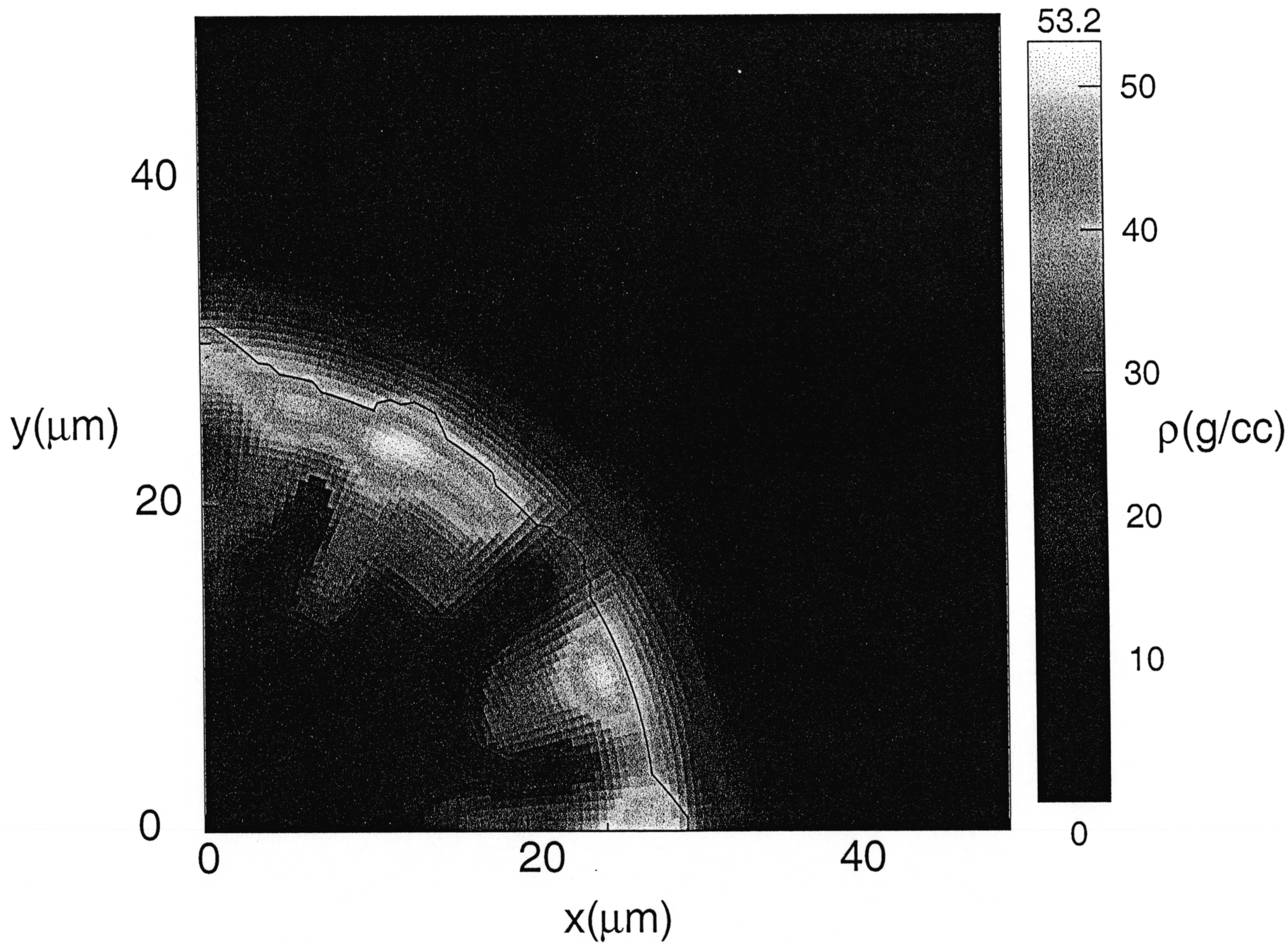



Fig. (1). The capsule consists of a plastic shell filled with DT gas. The plastic includes germanium to prevent hard x-rays from heating the inner portions of the shell. The inner layer of the plastic has a small amount of titanium mixed in. The fuel has a small amount of argon to serve as a spectroscopic tracer of conditions in the plastic.




The contour is the boundary of the region containing titanium

Fig. 2




The contour is the boundary of the region containing titanium

Fig. 3

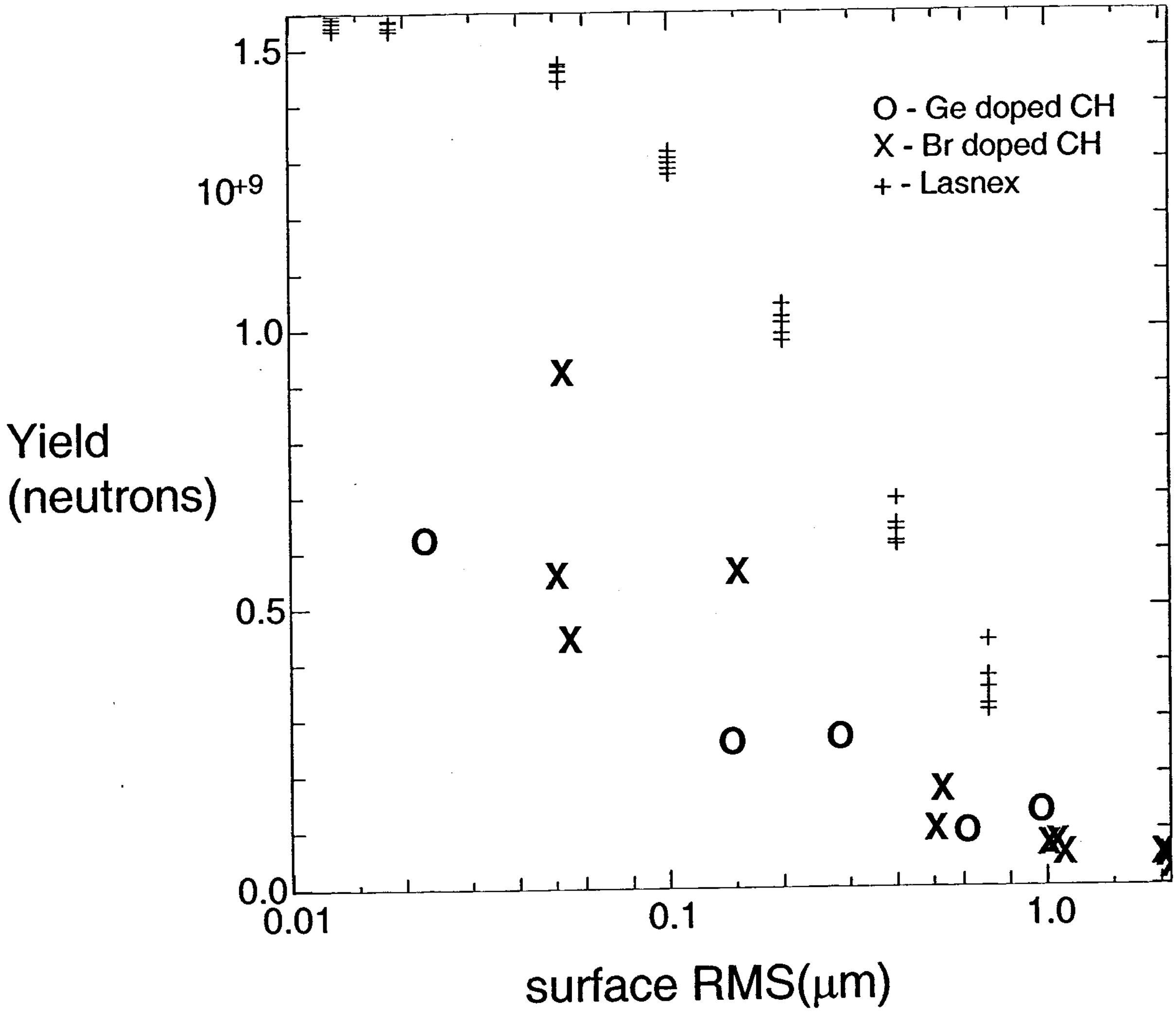

O - Ge doped CH
X - Br doped CH
+ - Lasnex
Yield
(neutrons)
$10^{+9}$
1.5
1.0
0.5
0.0
0.01
0.1
1.0
surface RMS(μm)

Fig. 4

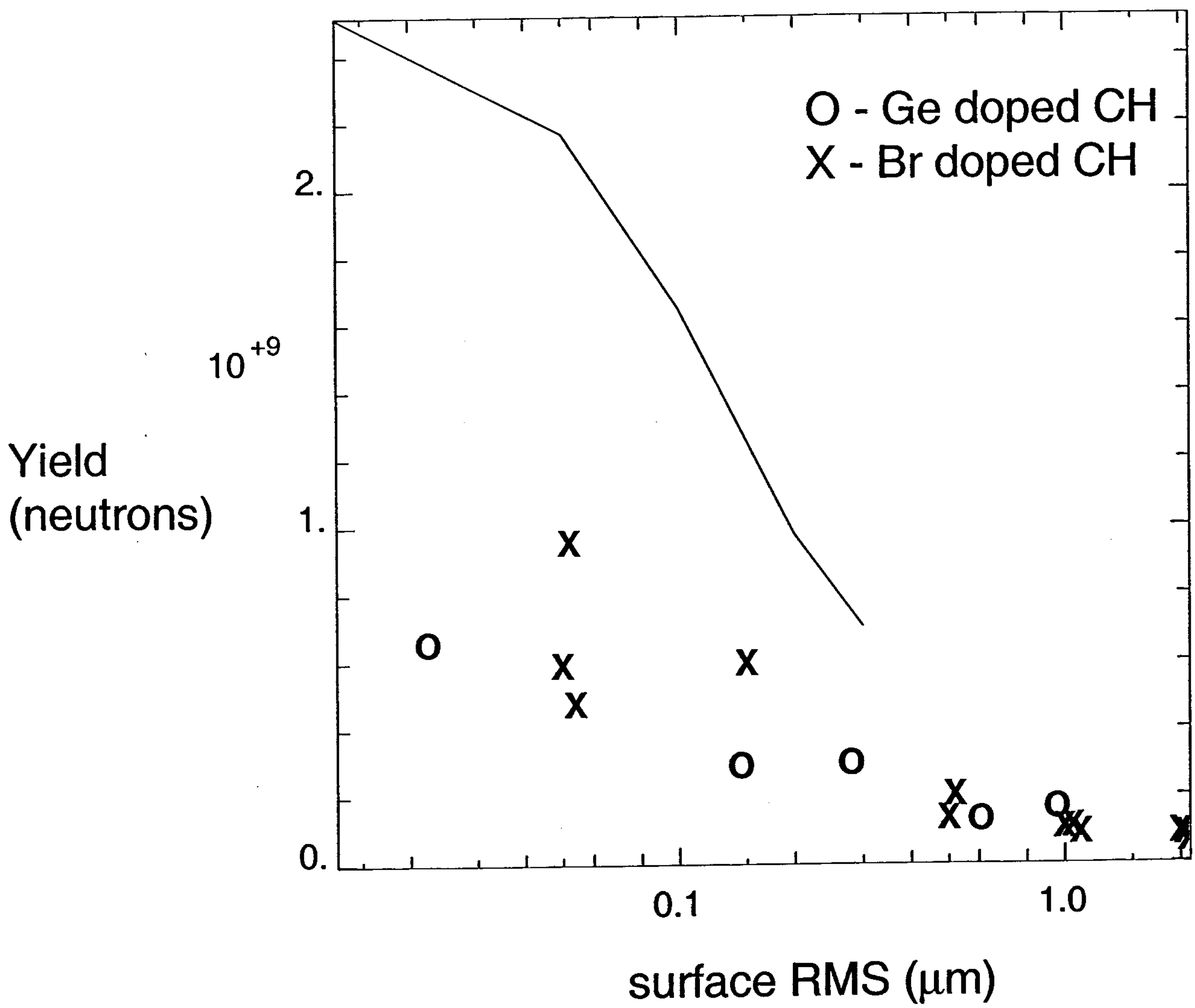
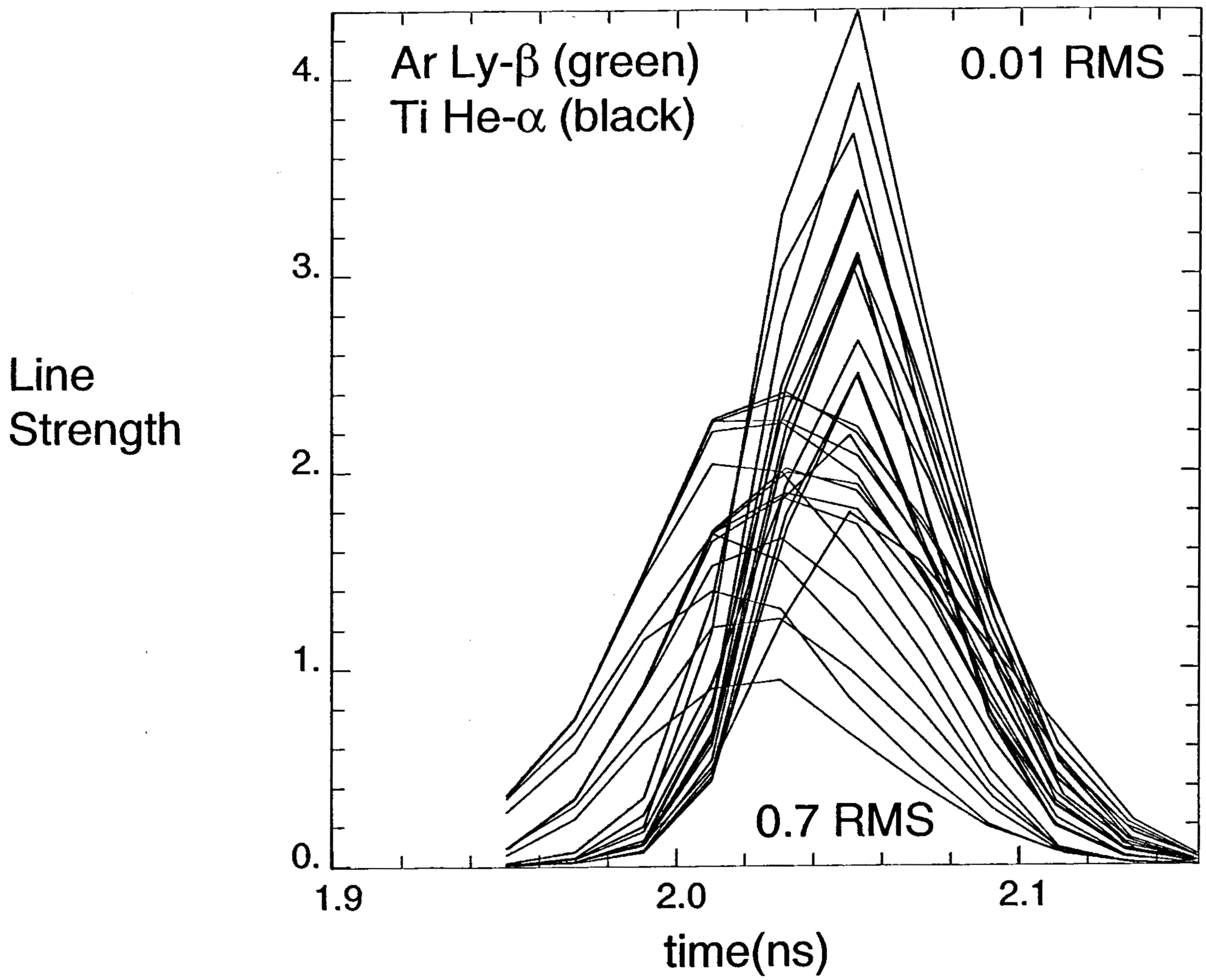
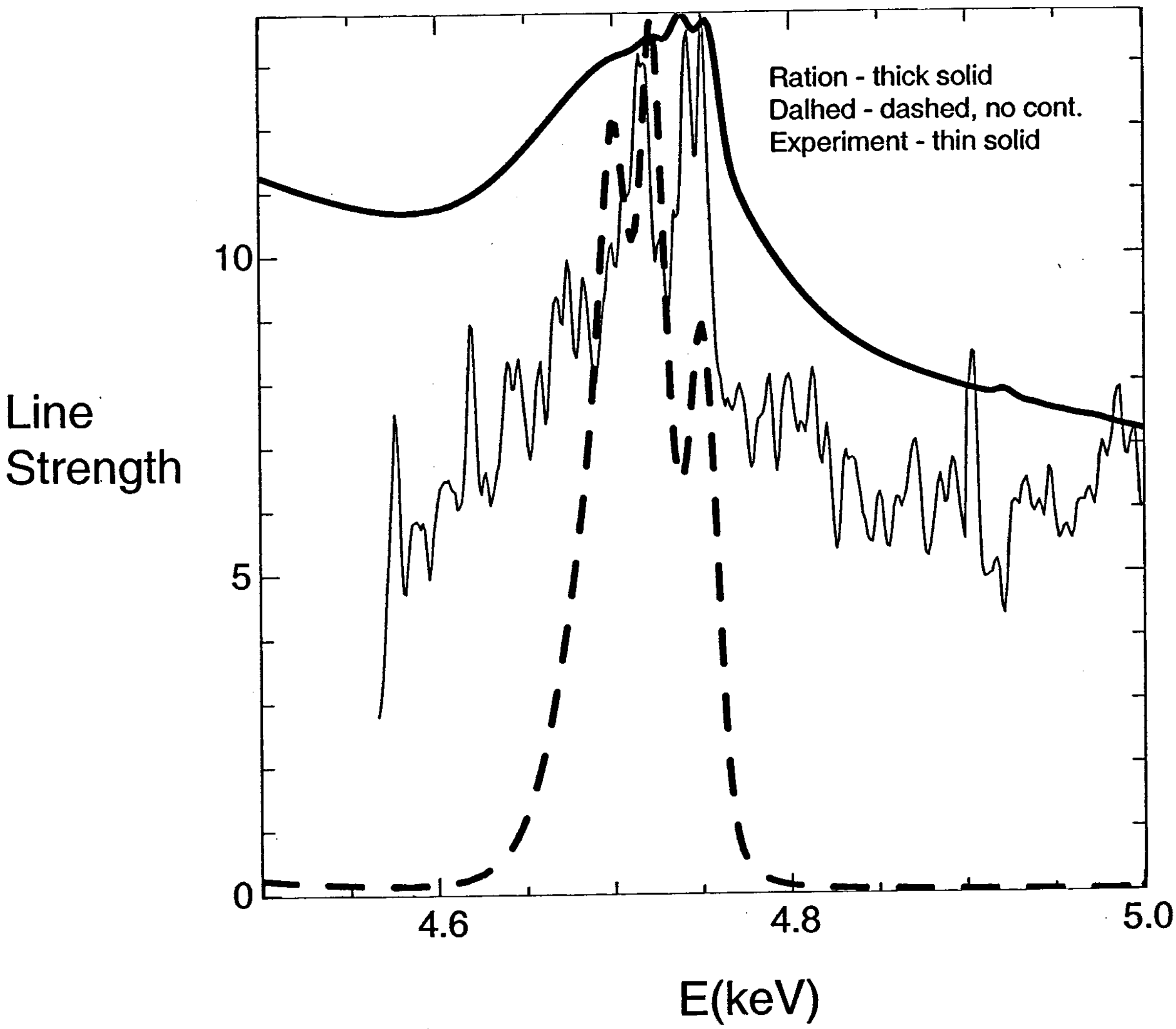

O - Ge doped CH
X - Br doped CH
2.
10^+9
Yield
(neutrons)
1.
0.
0.1
1.0
surface RMS (μm)

Fig. 5




Surface roughness= [0.01,0.02,0.05,0.1,0.2,0.4,0.7] μm RMS

Fig. 6



Ration - thick solid
Dalhed - dashed, no cont.
Experiment - thin solid
Line Strength
10
5
0
4.6
4.8
5.0
E(keV)


Fig. 7

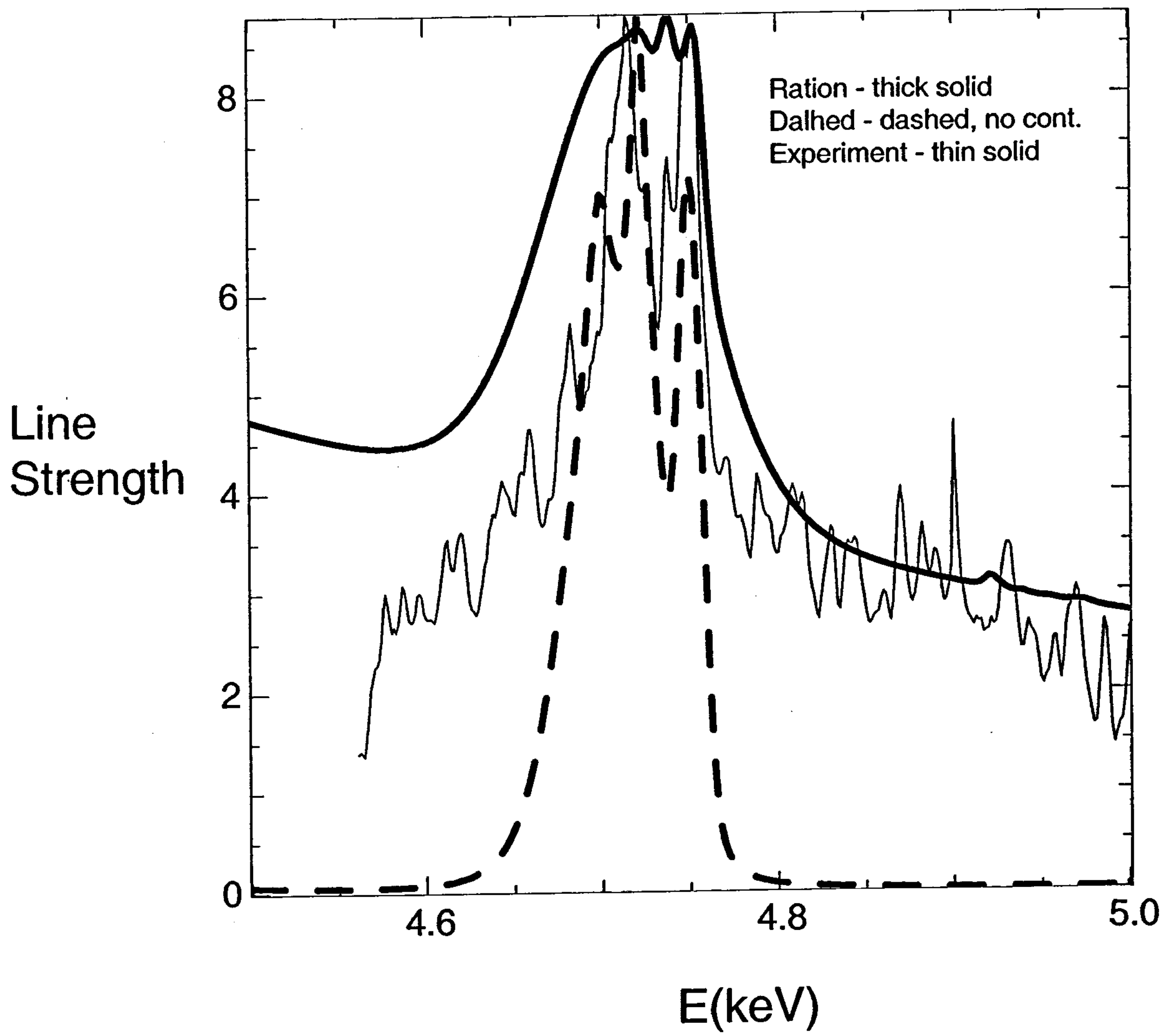

Ration - thick solid
Dalhed - dashed, no cont.
Experiment - thin solid
Line Strength
0
2
4
6
8
4.6
4.8
5.0
E(keV)

Fig. 8

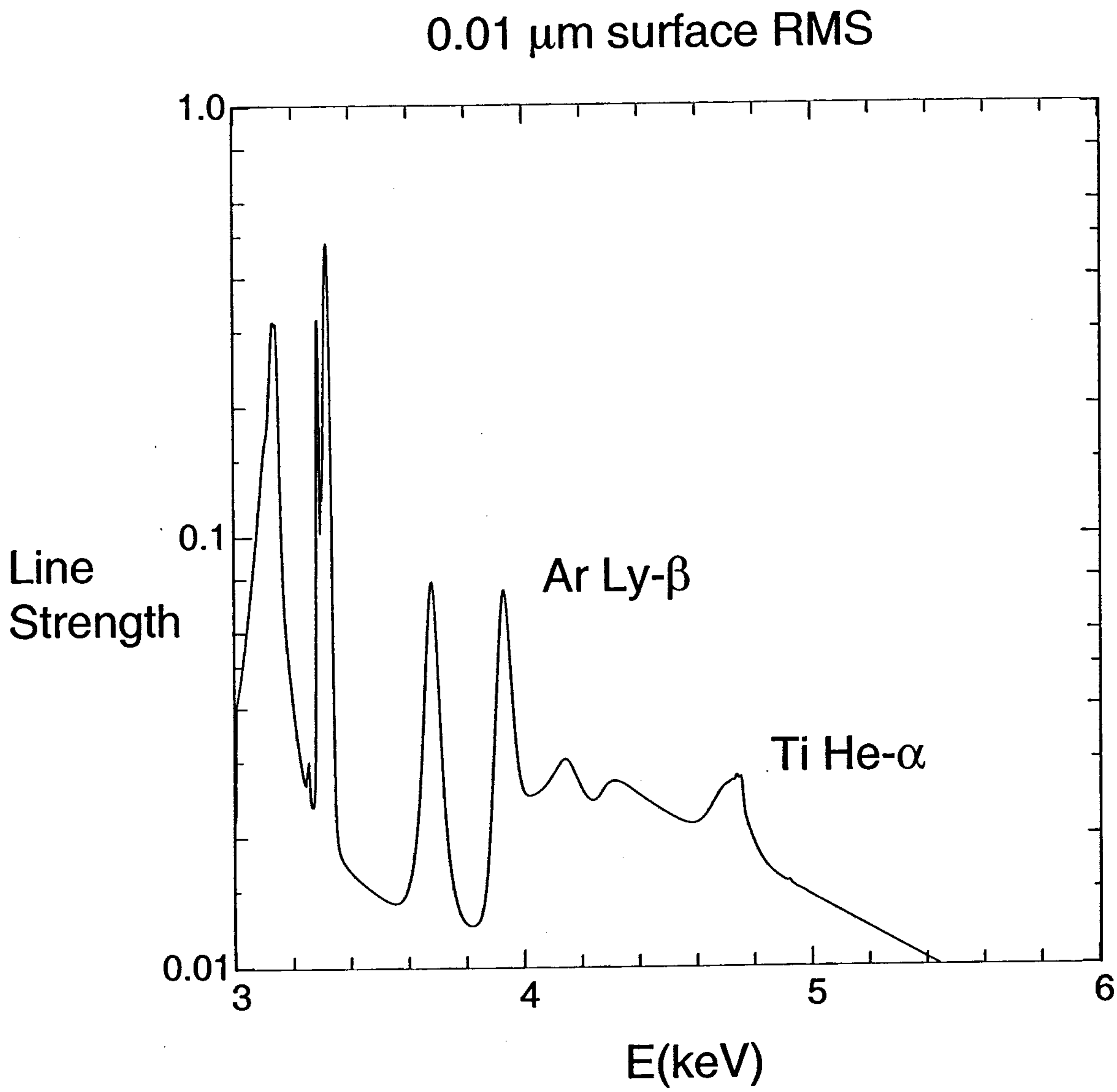

0.01 μm surface RMS
1.0
0.1
0.01
Line
Strength
Ar Ly-β
Ti He-α
3
4
5
6
E(keV)

Fig. 9

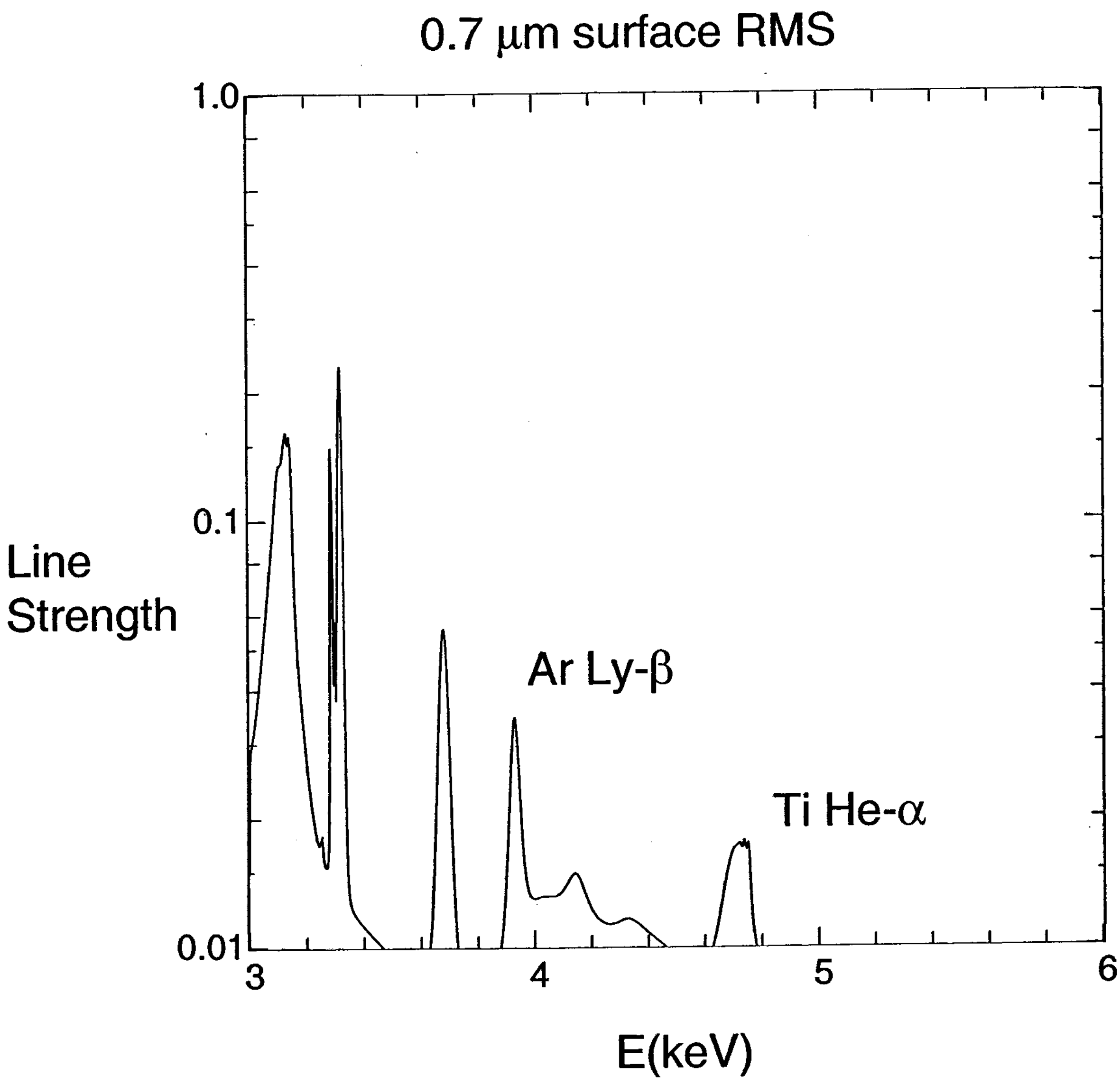
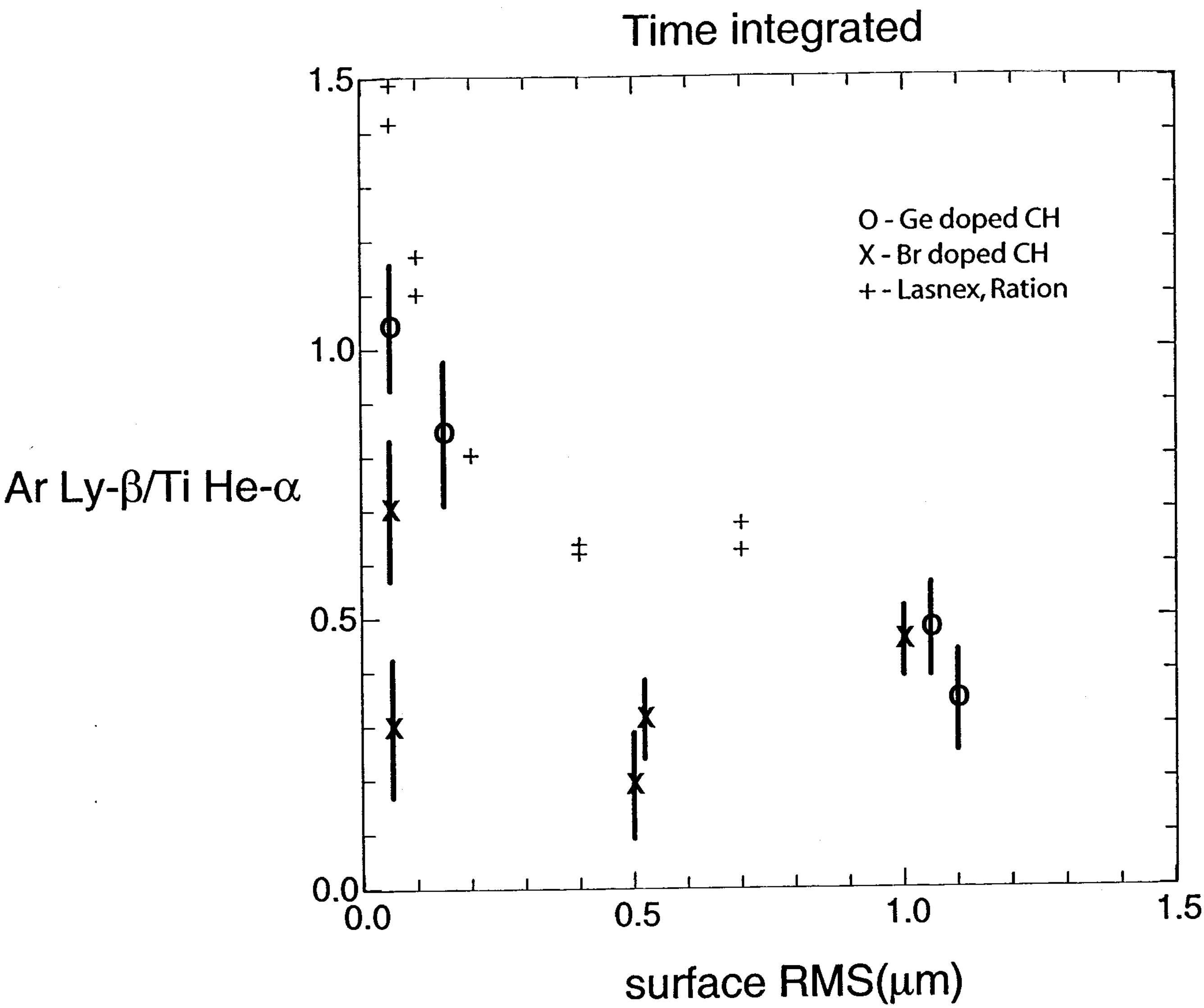

0.7 μm surface RMS
1.0
0.1
0.01
Line
Strength
Ar Ly-β
Ti He-α
3
4
5
6
E(keV)

Fig. 10



Time integrated
1.5
1.0
0.5
0.0
Ar Ly-β/Ti He-α
O - Ge doped CH
X - Br doped CH
+ - Lasnex, Ration
0.0
0.5
1.0
1.5
surface RMS(μm)


Fig. 11